

# Open Research Online

---

The Open University's repository of research publications and other research outputs

## Diffraction of a model set with complex windows

### Journal Item

#### How to cite:

Baake, Michael and Grimm, Uwe (2020). Diffraction of a model set with complex windows. Journal of Physics: Conference Series, 1458, article no. 012006.

For guidance on citations see [FAQs](#).

© 2020 Michael Baake; 2020 Uwe Grimm



<https://creativecommons.org/licenses/by/>

Version: Version of Record

Link(s) to article on publisher's website:

<http://dx.doi.org/doi:10.1088/1742-6596/1458/1/012006>

---

Copyright and Moral Rights for the articles on this site are retained by the individual authors and/or other copyright owners. For more information on Open Research Online's data [policy](#) on reuse of materials please consult the policies page.

---

[oro.open.ac.uk](http://oro.open.ac.uk)

PAPER • OPEN ACCESS

## Diffraction of a model set with complex windows

To cite this article: Michael Baake and Uwe Grimm 2020 *J. Phys.: Conf. Ser.* **1458** 012006

View the [article online](#) for updates and enhancements.

### Recent citations

- [On the \(dis\)continuity of the Fourier transform of measures](#)  
Timo Spindeler and Nicolae Strungaru
- [Inflation versus projection sets in aperiodic systems: the role of the window in averaging and diffraction](#)  
Michael Baake and Uwe Grimm



**IOP | ebooks™**

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

# Diffraction of a model set with complex windows

Michael Baake<sup>1</sup> and Uwe Grimm<sup>2</sup>

<sup>1</sup> Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany

<sup>2</sup> School of Mathematics and Statistics, The Open University, Milton Keynes MK7 6AA, UK

E-mail: mbaake@math.uni-bielefeld.de, uwe.grimm@open.ac.uk

**Abstract.** The well-known plastic number substitution gives rise to a ternary inflation tiling of the real line whose inflation factor is the smallest Pisot–Vijayaraghavan number. The corresponding dynamical system has pure point spectrum, and the associated control point sets can be described as regular model sets whose windows in two-dimensional internal space are Rauzy fractals with a complicated structure. Here, we calculate the resulting pure point diffraction measure via a Fourier matrix cocycle, which admits a closed formula for the Fourier transform of the Rauzy fractals.

Consider the primitive substitution  $\varrho$  defined by  $a \mapsto b \mapsto c \mapsto ab$  on the ternary alphabet  $\{a, b, c\}$ ; see [4, Ex. 4.4] for details. Its substitution matrix reads

$$M = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

with characteristic polynomial  $x^3 - x - 1$ . The latter is irreducible, with one real root,

$$\beta = \frac{(9 + \sqrt{69})^{\frac{1}{3}} + (9 - \sqrt{69})^{\frac{1}{3}}}{18^{\frac{1}{3}}} \approx 1.32472,$$

and a complex conjugate pair  $\alpha, \bar{\alpha}$  of algebraic conjugates, where  $|\alpha|^2 = \beta^{-1} = \beta^2 - 1$ . Below, we use  $\alpha$  for the number with positive imaginary part.

The algebraic integer  $\beta$  is a unit, and the smallest Pisot–Vijayaraghavan (PV) number, known as the *plastic number*; compare [4, p. 50 and Ex. 2.17]. It is also the Perron–Frobenius eigenvalue of  $M$ , where the corresponding left and right eigenvectors read

$$\langle u| = \frac{3 + \beta + 7\beta^2}{23}(1, \beta, \beta^2) \quad \text{and} \quad |v\rangle = (2 - \beta^2, \beta^2 - \beta, \beta - 1)^T,$$

which are strictly positive, and normalised such that  $\langle 1|v\rangle = \langle u|v\rangle = 1$ . So, the entries of  $|v\rangle$  are the relative frequencies of the letters in the symbolic sequences defined by  $\varrho$ , and  $P := |v\rangle\langle u|$  is a projector of rank 1, that is,  $P^2 = P$  and  $\text{image}(P) = \mathbb{R}|v\rangle$ .

To turn the symbolic sequences into tilings, we choose intervals of natural length, namely  $1, \beta$  and  $\beta^2$ , with control points on their left endpoints. For each sequence in the symbolic hull of  $\varrho$ , this leads to a typed point set,  $\Lambda = \Lambda_a \cup \Lambda_b \cup \Lambda_c$ , from the three types of control



points. The average distance between neighbouring points in  $\Lambda$  is  $\bar{s} = 4 + 2\beta - 3\beta^2$ , so we get  $\text{dens}(\Lambda) = 1/\bar{s} = \frac{1}{23}(3 + \beta + 7\beta^2)$  and  $\text{dens}(\Lambda_i) = v_i \text{dens}(\Lambda)$  for  $i \in \{a, b, c\}$ .

To continue, we work with the rank-3  $\mathbb{Z}$ -module  $L = \mathbb{Z}[\beta] = \langle 1, \beta, \beta^2 \rangle_{\mathbb{Z}}$ , which comprises all possible coordinates of our control points (relative to one of them, then considered as 0). The Minkowski embedding [4, Ex. 3.5] of  $L$  is a lattice  $\mathcal{L}$  in  $\mathbb{R} \times \mathbb{C} \simeq \mathbb{R}^3$ , with  $\text{dens}(\mathcal{L}) = 2/\sqrt{23}$ . A canonical choice for the basis matrix of  $\mathcal{L}$  and its dual,  $\mathcal{L}^*$ , is

$$\mathcal{B} = \begin{pmatrix} 1 & \beta & \beta^2 \\ 1 & \text{Re}(\alpha) & \text{Re}(\alpha^2) \\ 0 & \text{Im}(\alpha) & \text{Im}(\alpha^2) \end{pmatrix} \quad \text{and} \quad \mathcal{B}^* = \frac{2}{\sqrt{23}} \begin{pmatrix} \text{Im}(\alpha)\beta^{-1} & \text{Im}(\alpha)\beta & \text{Im}(\alpha) \\ 2\text{Im}(\alpha)\beta^2 & -\text{Im}(\alpha)\beta & -\text{Im}(\alpha) \\ \beta & -1 + \frac{3}{2}\beta^2 & -\frac{3}{2}\beta \end{pmatrix},$$

where  $\text{Re}(\alpha) = -\beta/2$ ,  $\text{Re}(\alpha^2) = 1 - \beta^2/2$ ,  $\text{Im}(\alpha) = \frac{4+9\beta-6\beta^2}{2\sqrt{23}}$  and  $\text{Im}(\alpha^2) = \frac{6+2\beta-9\beta^2}{2\sqrt{23}}$  in our setting. We note in passing that duality can also be defined via the quadratic form  $(x, y) := xy + \text{Re}(\sigma(x)\overline{\sigma(y)})$ , where  $\sigma : \mathbb{Q}(\beta) \rightarrow \mathbb{Q}(\alpha)$  denotes the algebraic conjugation map  $\sigma$  defined by  $\beta \mapsto \alpha$  and its unique extension to a field isomorphism.

We can extract the *Fourier module* from the first line of the dual basis matrix  $\mathcal{B}^*$  as

$$L^{\otimes} = \frac{2\text{Im}(\alpha)}{\beta\sqrt{23}} \langle 1, \beta^2, \beta \rangle_{\mathbb{Z}} = \frac{5 - 6\beta + 4\beta^2}{23} L, \quad (1)$$

which is also the dynamical spectrum (in additive notation) of the tiling dynamical system as well as the (topologically equivalent) model set dynamical system defined by the control point sets; see [6] for background. Our system has pure point diffraction spectrum, because the defining point set is a regular model set (see below).

The Bragg peaks can be indexed by three integer Miller indices  $(n_0, n_1, n_2)$ , where we parameterise the wave number, in line with (1), as

$$k = k(n_0, n_1, n_2) = \frac{5 - 6\beta + 4\beta^2}{23} (n_0 + n_1\beta + n_2\beta^2). \quad (2)$$

The original version of the Minkowski embedding of  $\mathbb{Z}[\beta]$  uses complex numbers, which is natural from an algebraic perspective. However, for Fourier analysis, we better work with real numbers, via  $\mathbb{C} \simeq \mathbb{R}^2$ , as initiated above for  $\mathcal{B}$  and  $\mathcal{B}^*$ . Given the conjugation map  $\sigma$ , the  $\star$ -map:  $\mathbb{Q}(\beta) \rightarrow \mathbb{R}^2$  is conveniently defined by  $x \mapsto (\text{Re}(\sigma(x)), \text{Im}(\sigma(x)))^T$ . If  $k \in L^{\otimes}$  is parameterised as in (2), this means

$$k^{\star} = \begin{pmatrix} \frac{1}{46}((18n_0 - 4n_1 + 6n_2) + (6n_0 - 9n_1 + 2n_2)\beta - (4n_0 - 6n_1 + 9n_2)\beta^2) \\ \frac{1}{2\sqrt{23}}(2n_2 + (3n_1 - 2n_0)\beta - 3n_2\beta^2) \end{pmatrix}.$$

Next, we need the displacement (or digit) matrix  $T$  of our inflation rule in direct space; see [1] for definitions and properties. With the interval lengths as chosen above, it reads

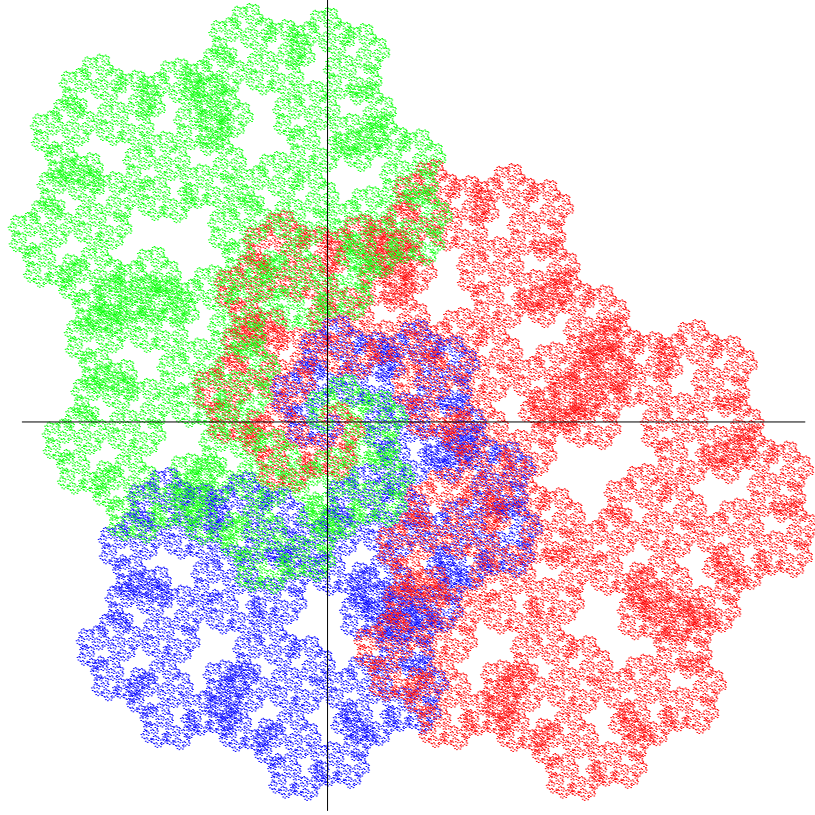
$$T = \begin{pmatrix} \emptyset & \emptyset & \{0\} \\ \{0\} & \emptyset & \{1\} \\ \emptyset & \{0\} & \emptyset \end{pmatrix},$$

which is also reflected in the point set iteration

$$\Lambda'_a = \beta\Lambda_c, \quad \Lambda'_b = \beta\Lambda_a \cup (\beta\Lambda_c + 1), \quad \Lambda'_c = \beta\Lambda_b.$$

It is known that we obtain a regular model set [10], with three topologically regular windows that have disjoint interiors. They are compact sets  $W_a, W_b, W_c \subset \mathbb{C}$  that satisfy

$$W_a = \alpha W_c, \quad W_b = \alpha W_a \cup (\alpha W_c + 1), \quad W_c = \alpha W_b. \quad (3)$$



**Figure 1.** Illustration of the three windows  $W_a$  (blue),  $W_b$  (red) and  $W_c$  (green) of the plastic number inflation rule. For a more detailed version of  $W_b$  and further properties, see [4, Fig. 7.3].

This defines a contractive iterated function system (IFS), so that the fixed point (and hence our window triple) is unique. Due to the nature of  $\Lambda$  and  $\Lambda_i$  as regular model sets, the volumes (areas) of the windows, compare [4, Ex. 7.6 and Fig. 7.3], satisfy the relations  $\text{dens}(\mathcal{L}) \text{vol}(W_i) = v_i \text{dens}(\Lambda)$ , which results in the values

$$\text{Im}(\alpha)(\beta^2 - 1, \beta, 1) = \frac{1}{2\sqrt{23}} (5 - 6\beta + 4\beta^2, -6 - 2\beta + 9\beta^2, 4 + 9\beta - 6\beta^2).$$

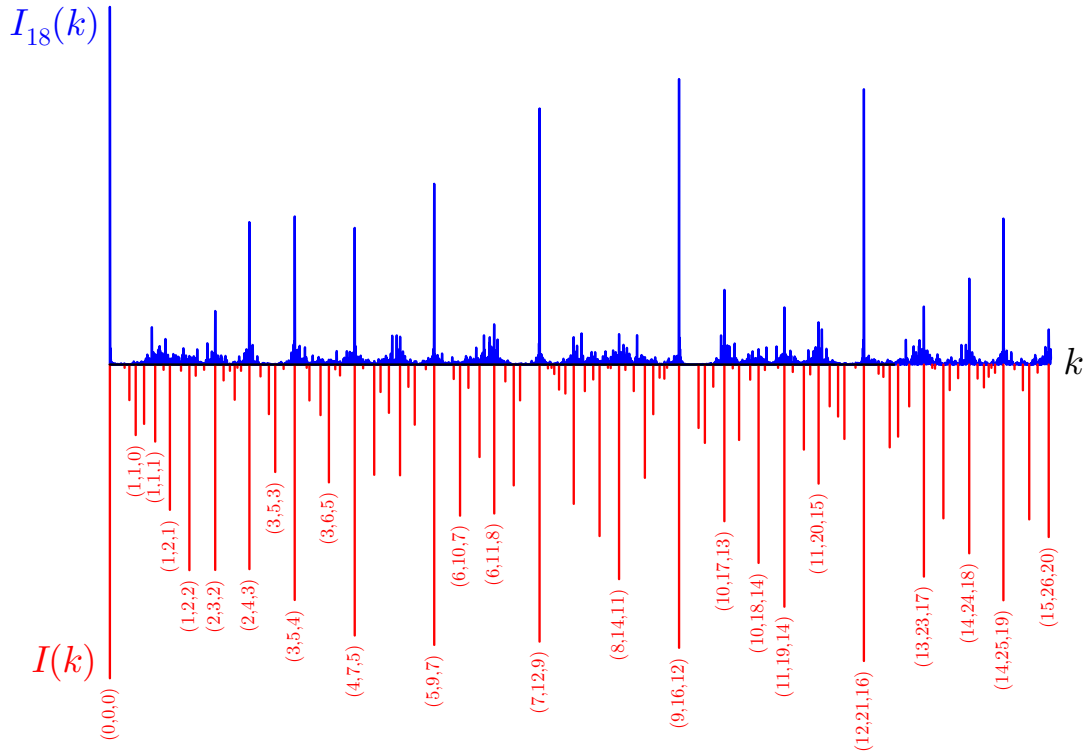
The three windows are complex Rauzy fractals with a complicated topological structure [9]; see Figure 1 for an illustration and [8, Sec. 7.4] and references therein for background on Rauzy fractals. From the general diffraction result for regular model sets, see [4] and references therein, the weighted Dirac comb  $\omega = \sum_{i \in \{a,b,c\}} h_i \delta_{\Lambda_i}$  with  $h_i \in \mathbb{C}$  has diffraction

$$\widehat{\gamma_\omega} = \sum_{k \in L^\otimes} I(k) \delta_k \quad \text{with} \quad I(k) = \left| \sum_i h_i A_i(k) \right|^2, \quad (4)$$

because the Bombieri–Taylor property holds for primitive inflation rules [3, Rem. 3.24]. Here, setting  $W = W_a \cup W_b \cup W_c$ , the amplitudes are given by

$$A_i(k) = \frac{\text{dens}(\Lambda_i)}{\text{vol}(W_i)} \widetilde{1_{W_i}}(k^\star) = \frac{\text{dens}(\Lambda)}{\text{vol}(W)} \widetilde{1_{W_i}}(k^\star),$$

where  $1_K$  denotes the characteristic function of the set  $K$ . Though this formula looks nice, it is difficult to calculate  $\widetilde{1_{W_i}}$  directly, due to the fractal nature of the window boundaries. Let us next explain an alternative approach that harvests the inflation nature of our point sets.



**Figure 2.** Bragg peaks of the plastic number inflation rule (red, bottom; some with their Miller index triple) as obtained from the cocycle approach, in comparison with a finite-size approximation by exponential sums (blue, top).

We start by reformulating the window IFS (3) in  $\mathbb{R}^2$ . Recall that multiplication with  $\alpha \in \mathbb{C}$  is matrix multiplication with  $\underline{Q} = \begin{pmatrix} \operatorname{Re}(\alpha) & -\operatorname{Im}(\alpha) \\ \operatorname{Im}(\alpha) & \operatorname{Re}(\alpha) \end{pmatrix}$  in  $\mathbb{R}^2$ , where  $\det(\underline{Q}) = |\alpha|^2 = \beta^{-1}$ . As the windows are interior-disjoint, Eq. (3) turns into equations in  $L^1(\mathbb{R}^2)$  for the characteristic functions of the windows and their images. Setting  $f_i(y) := \widetilde{1_{W_i}}(y)$  and using the relation

$$\widetilde{1_{AK+t}}(y) = |\det(A)| e^{2\pi i \langle t|y \rangle} \widetilde{1_K}(A^T y),$$

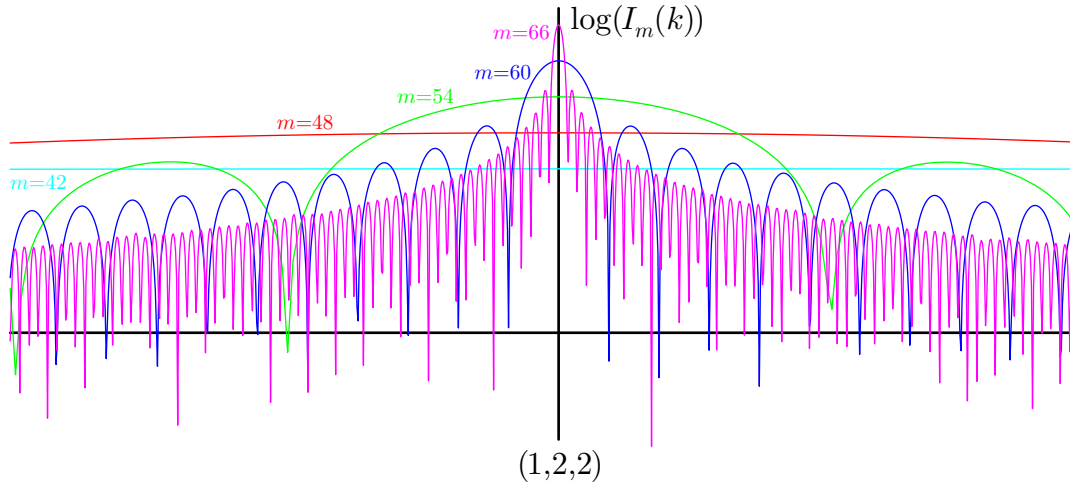
which holds for any real, invertible  $2 \times 2$ -matrix  $A$  and compact set  $K \subset \mathbb{R}^2$ , one finds

$$\begin{pmatrix} f_a \\ f_b \\ f_c \end{pmatrix}(y) = \beta^{-1} \underline{B}(y) \begin{pmatrix} f_a \\ f_b \\ f_c \end{pmatrix}(\underline{R}y), \quad \text{with } \underline{R} = \underline{Q}^T \text{ and } \underline{B}(y) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & e^{2\pi i y_1} \\ 0 & 1 & 0 \end{pmatrix}. \quad (5)$$

Here,  $\underline{B}(y)$  is the *internal Fourier matrix* that emerges from the (inverse) Fourier transform of the  $\star$ -image of  $T$ , that is,  $\underline{B}_{ij}(y) = \sum_{x \in T_{ij}} e^{2\pi i \langle x^* | y \rangle}$ , where  $y \in \mathbb{R}^2$ .

Now, for  $n \in \mathbb{N}$ , we can define a cocycle via  $\underline{B}^{(n)}(y) = \underline{B}(y) \underline{B}(\underline{R}y) \cdots \underline{B}(\underline{R}^{n-1}y)$ , with  $\underline{B}^{(1)} = \underline{B}$  and  $\underline{B}^{(n)}(0) = M^n$ . Next, consider the matrix function  $C(y) := \lim_{n \rightarrow \infty} \beta^{-n} \underline{B}^{(n)}(y)$ , which is well defined because the limit exists for every  $y \in \mathbb{R}^2$ . In fact,  $C$  is a continuous matrix function, and one has

$$C(0) = P = |v\rangle\langle u| = \frac{3 + \beta + 7\beta^2}{23} \begin{pmatrix} 2 - \beta^2 & \beta - 1 & \beta^2 - \beta \\ \beta^2 - \beta & 1 + \beta - \beta^2 & \beta^2 - 1 \\ \beta - 1 & \beta^2 - \beta & 1 + \beta - \beta^2 \end{pmatrix}.$$



**Figure 3.** Example of a Bragg peak and its successive approximations, for wave numbers  $k \in [1.2672395, 1.2672405]$  and finite systems defined by the point sets from the inflation words  $q^m(a)$  with  $m \in \{42, 48, 54, 60, 66\}$ . The vertical black line denotes the location of the Bragg peak  $(1, 2, 2)$ . Note that, to be able to compare different system sizes, the logarithm of the intensity is plotted.

Moreover, one can show that  $C(y) = |c(y)\rangle\langle u|$  with  $|c(0)\rangle = |v\rangle$  and  $|f(y)\rangle = \frac{\text{dens}(\Lambda)}{\text{dens}(\mathcal{L})} |c(y)\rangle$ . In particular, one has  $|c(y)\rangle = C(y)|v\rangle$ , which makes the functions  $f_i$  accessible.

For  $k \in L^\otimes$  and  $i \in \{a, b, c\}$ , our amplitudes are

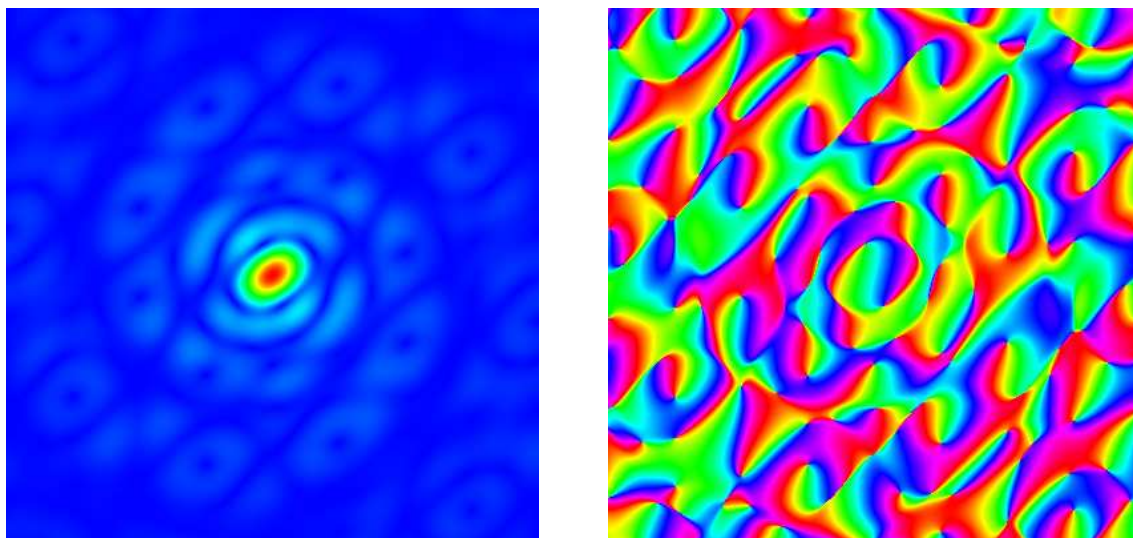
$$A_i(k) = \text{dens}(\Lambda) c_i(k^*) = \frac{3 + \beta + 7\beta^2}{23} c_i(k^*),$$

and the corresponding intensities follow from Eq. (4). For any index triple, the intensity at the corresponding wave number  $k \in L^\otimes$  is approximated by truncating the infinite product representation for  $C(k^*)$  and calculating the amplitudes as explained above. Here, by using about 50–100 terms, one obtains the peaks with a relative precision better than  $10^{-10}$ .

Since the diffraction measure  $\widehat{\gamma_\omega}$  can also be approximated (in the vague topology) by the absolute squares of exponential sums of finite approximants (divided by the system size), we illustrate the diffraction of the uniform Dirac comb (all  $h_i = 1$ ) in Figure 2 in comparison to an approximation for a finite system with 114 tiles, obtained by  $m = 18$  inflation steps from an initial tile of type  $a$ . Here, as well as in Figure 3, the function  $I_m(k)$  for the approximation refers to the (absolutely continuous) diffraction intensity for the corresponding finite system. The apparent mismatch emerges from the extremely slow convergence of the finite-size approximation, which should not come as a surprise due to the complicated fractal nature of the windows. To expand on the latter, we compare the neighbourhood of the peak with Miller indices  $(1, 2, 2)$  at  $k = (1 + 8\beta + 10\beta^2)/23 \approx 1.267240014$  with approximations for various system sizes in Figure 3.

While the computation of the spectrum requires that  $k \in L^\otimes$ , the recursion equations (5) for the (inverse) Fourier transforms of the three windows can be used for any  $y \in \mathbb{R}^2$ . Thus, the (inverse) Fourier transform of the windows can be computed efficiently, despite the complex nature of the windows. As an example, the inverse Fourier transform  $f_b = 1_{W_b}$  of the largest window is shown in Figure 4. In general, it is difficult to compute the Fourier transform of fractals; see, for instance, [7] for a related result on self-similar fractals of zero Lebesgue measure.





**Figure 4.** Inverse Fourier transform  $f_b(y)$  of the window  $W_b$  for  $y \in [-4, 4]^2$ . The left panel shows the absolute value, which takes values between 0 (blue) and  $f_b(0) = \text{vol}(W_b) = v_2 = \beta^2 - \beta$  (red). The right panel shows the corresponding argument (with red representing phase 0).

The cocycle method explained for this example works in full generality for all primitive PV inflation rules (with a unit inflation factor) that lead to regular model sets. In fact, it can even be applied to any primitive PV inflation rule, as well as to  $S$ -adic inflations with the same PV inflation multiplier and compatible tile sizes. When the spectrum is mixed, the cocycle method reproduces the pure point part; further details will be given in a forthcoming publication [5].

### Acknowledgments

It is our pleasure to thank the MFO at Oberwolfach for hospitality, where this manuscript was completed. Our work was supported by the German Research Foundation (DFG), within the CRC 1283 at Bielefeld University, and by EPSRC through grant EP/S010335/1.

### References

- [1] Baake M, Frank N P, Grimm U and Robinson E A 2019 Geometric properties of a binary non-Pisot inflation and absence of absolutely continuous diffraction *Studia Math.* **247** 109–154 (*Preprint* arXiv:1706.03976)
- [2] Baake M and Gähler F 2016 Pair correlations of aperiodic inflation rules via renormalisation: Some interesting examples *Topology & Appl.* **205** 4–27 (*Preprint* arXiv:1511.00885)
- [3] Baake M, Gähler F and Mañibo N 2019 Renormalisation of pair correlation measures for primitive inflation rules and absence of absolutely continuous diffraction *Commun. Math. Phys.* in press (*Preprint* arXiv:1805.09650)
- [4] Baake M and Grimm U 2013 *Aperiodic Order. Vol. 1: A Mathematical Invitation* (Cambridge: Cambridge University Press)
- [5] Baake M and Grimm U 2019 Fourier transform of Rauzy fractals and the point spectrum of Pisot inflation tilings (in preparation)
- [6] Baake M and Lenz D 2018 Spectral notions of aperiodic order *Discr. Cont. Dynam. Syst. S* **10** 161–190 (*Preprint* arXiv:1601.06629)
- [7] Dettmann C P and Frankel N E 1993 Structure factor of deterministic fractals with rotations *Fractals* **1** 253–261
- [8] Pytheas Fogg N 2002 *Substitutions in Dynamics, Arithmetics and Combinatorics* LNM 1794 (Berlin: Springer)
- [9] Siegel A and Thuswaldner J M 2009 *Topological Properties of Rauzy Fractals* Mém. Soc. Math. France 118 (Paris: Société Mathématiques de France)
- [10] Sing B 2007 *Pisot Substitutions and Beyond* PhD thesis (Bielefeld: Bielefeld University) available electronically at <https://pub.uni-bielefeld.de/publication/2302336>